ROYAL INSTITUTE OF TECHNOLOGY

Numerical simulation of breakup of small aggregates in turbulence

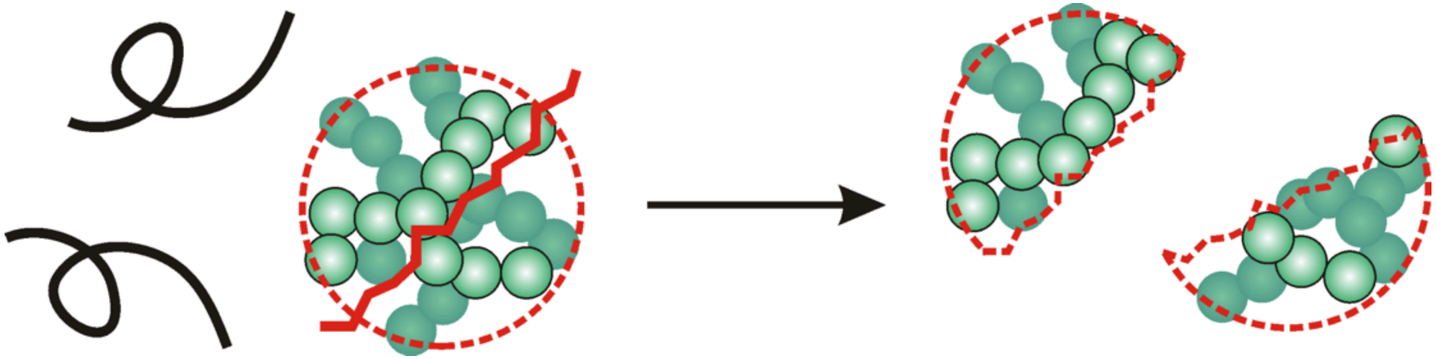
Matthäus U. Bäbler
Dept. Chemical Engineering and Technology, KTH, Stockholm, Sweden

Luca Biferale
Dept. Physics and INFN, University of Rome Tor Vergata, Italy

Alessandra S. Lanotte
ISAC-CNR and INFN, Sez. Lecce, Italy

ECCE10 - 10th European Congress of Chemical Engineering
Nice, September 27 to October 1, 2015

Breakup of aggregates



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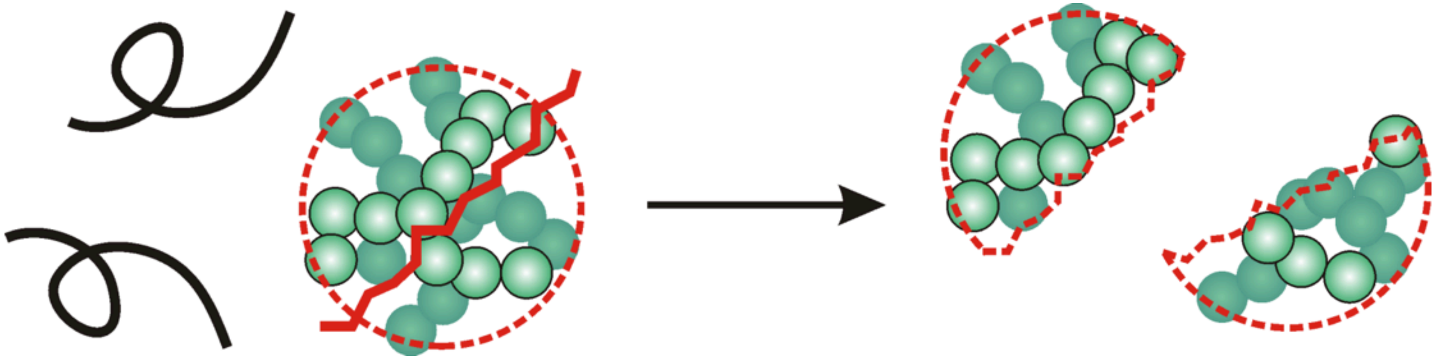
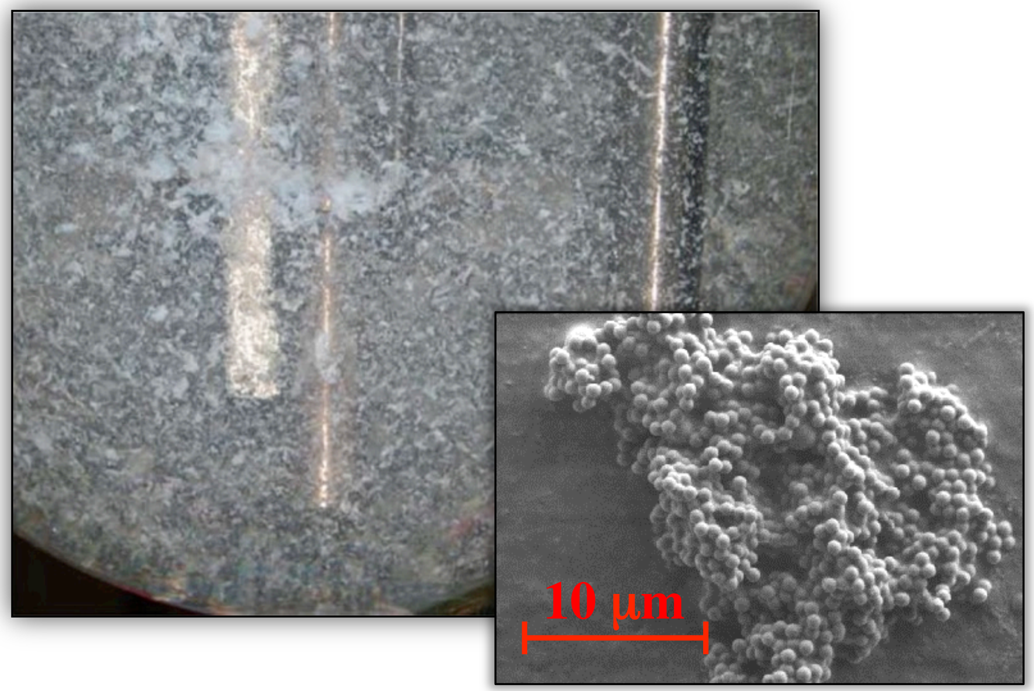
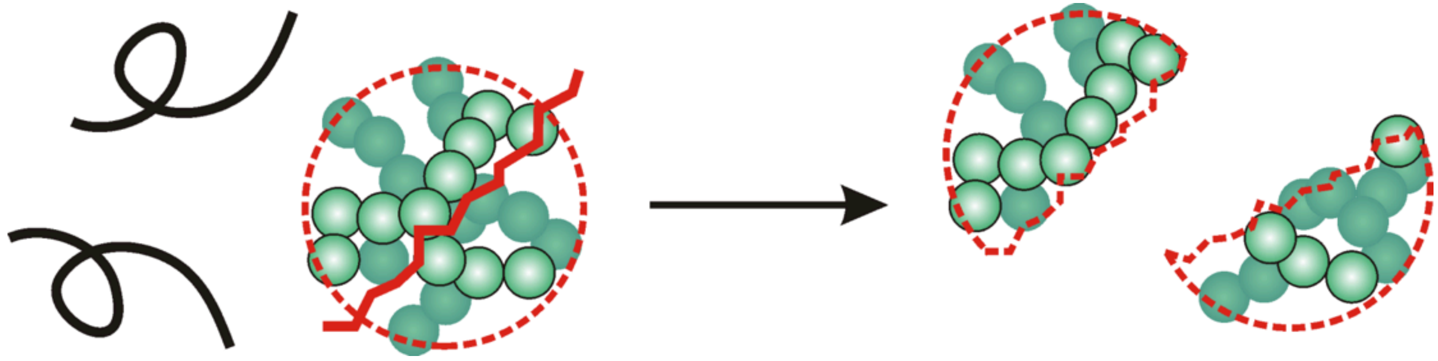


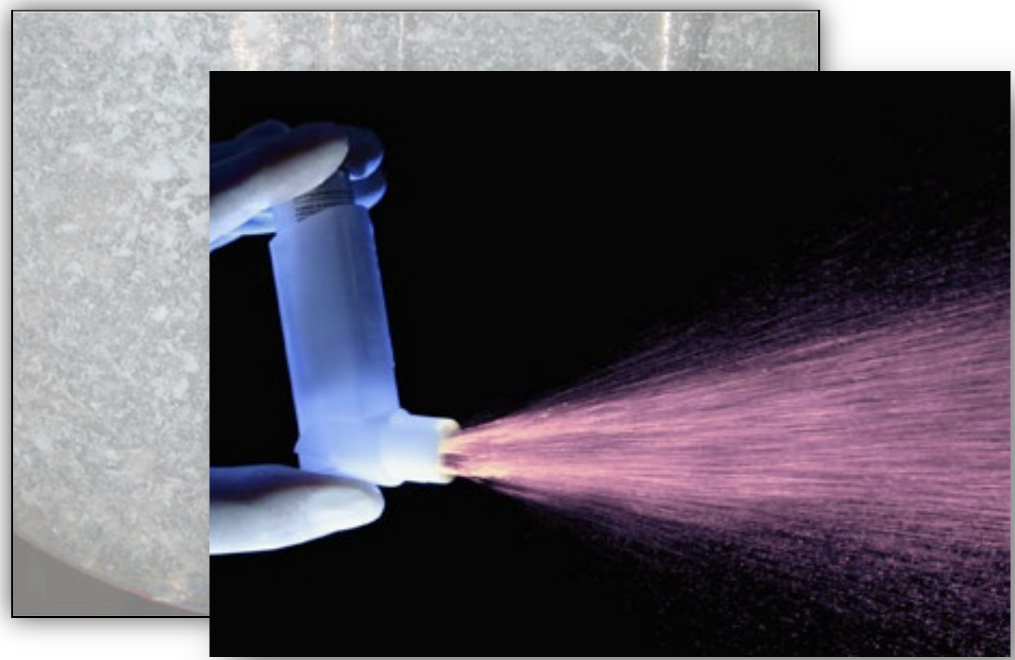


- Processing of industrial colloids (polymers, metal oxides, minerals)

Pictures: M. Soos, D. Marchisio, J. Sefcik, *AIChE J.* (2013) and Soos, et al., *J. Colloid Interface Sci.* (2008)

Breakup of aggregates

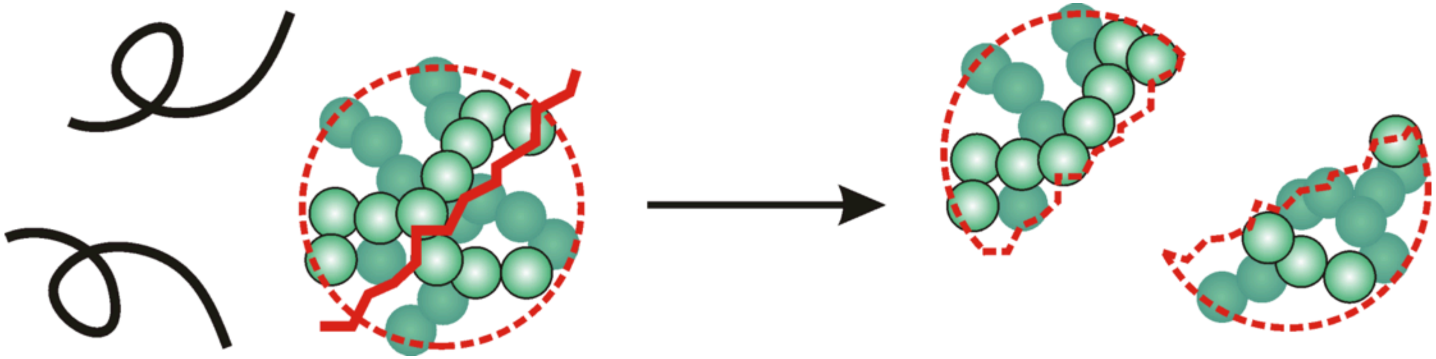




- Processing of industrial colloids (polymers, metal oxides, minerals)
- Dispersion of powder agglomerates for, e.g. inhalation drugs

Picture: Getty images (2015-03-22)

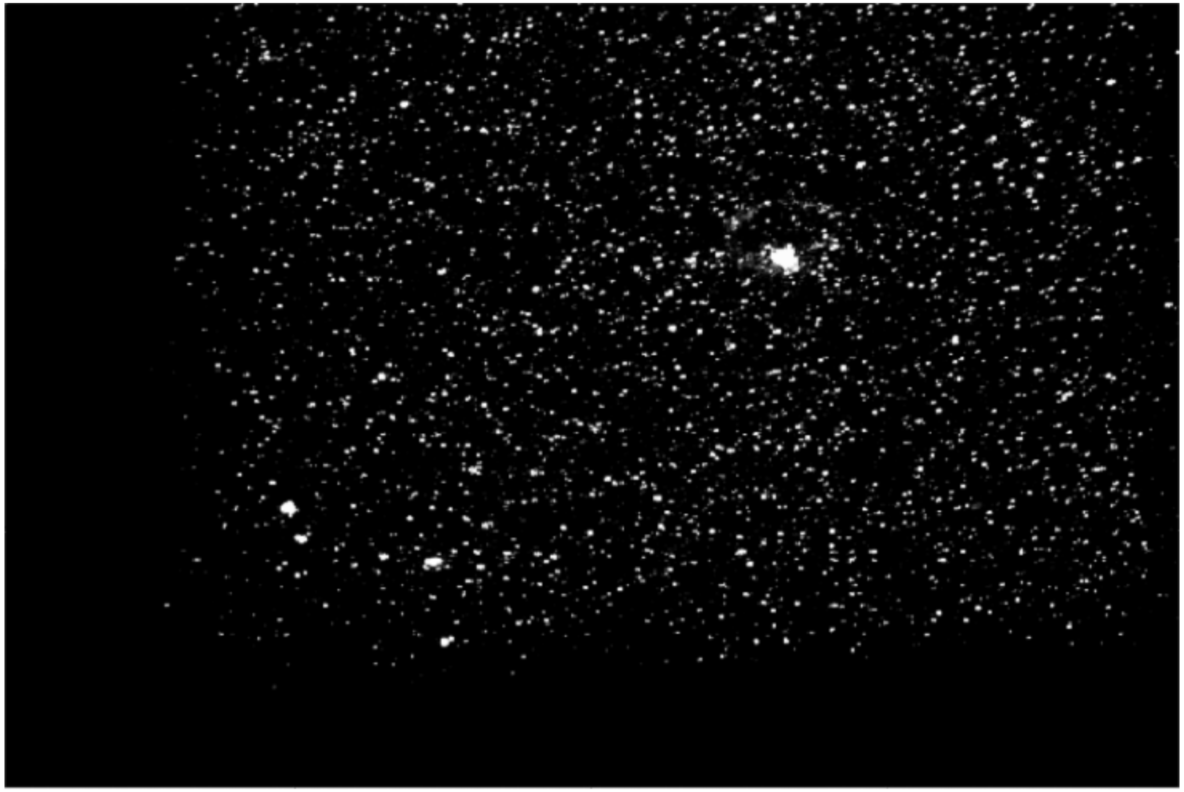
Breakup of aggregates



- Processing of industrial colloids (polymers, metal oxides, minerals)
- Dispersion of powder agglomerates for, e.g. inhalation drugs
- Evolution and transport of sediments and suspended mater in natural waters

Picture: Satelite image Rio de la Plata Estuary, March 10, 2010 (www.eosnap.com, retrieved 2014-03-12),

Breakup of aggregates

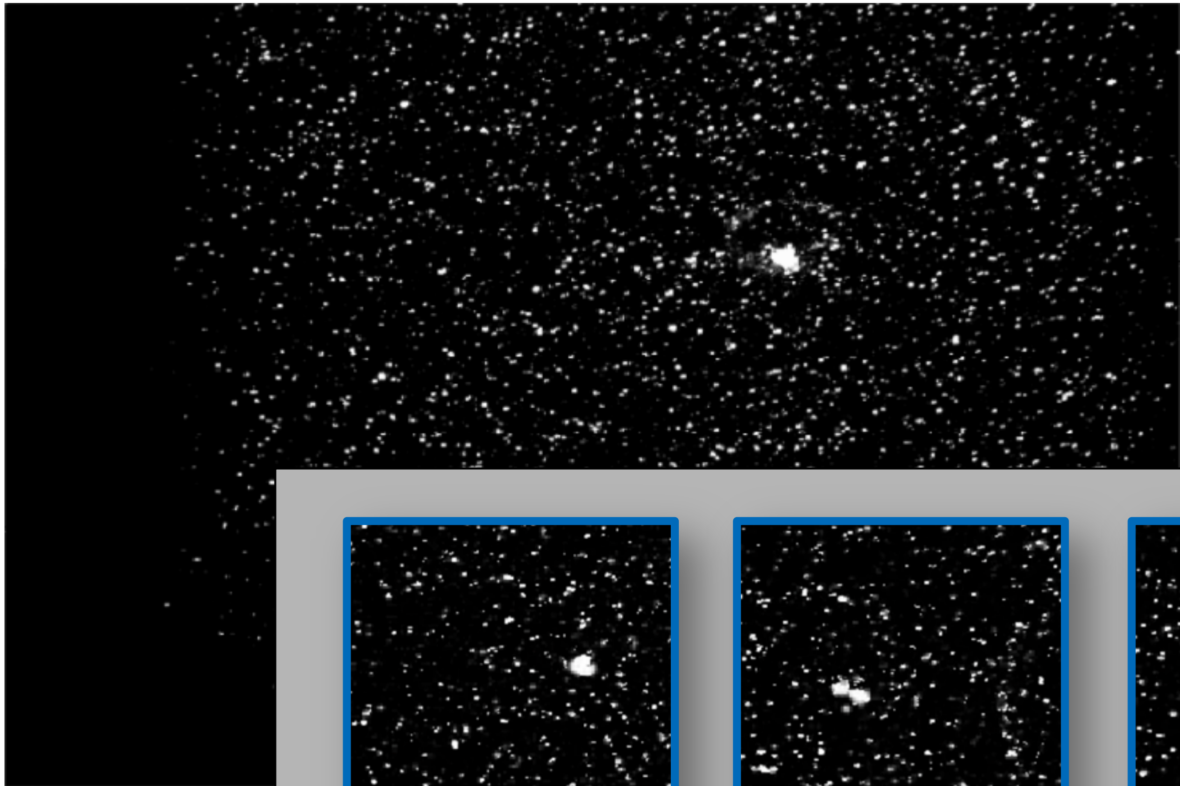


Breakup of a polystyrene aggregate in homogeneous and isotropic turbulence, monitored by 3D-Particle Tracking Velocimetry.

$$Re_\lambda \approx 117$$
$$\eta = 0.15\,\mathrm{mm}$$
$$\tau_\eta = 0.02\,\mathrm{s}$$
$$d_{\mathrm{agg}} = 1\,\mathrm{mm}$$

D. Saha, M.U. Bäbler, M. Holzner, M. Soos, B. Lüthi, A. Liberzon, W. Kinzelbach, *submitted to Langmuir* (2015)

Breakup of aggregates



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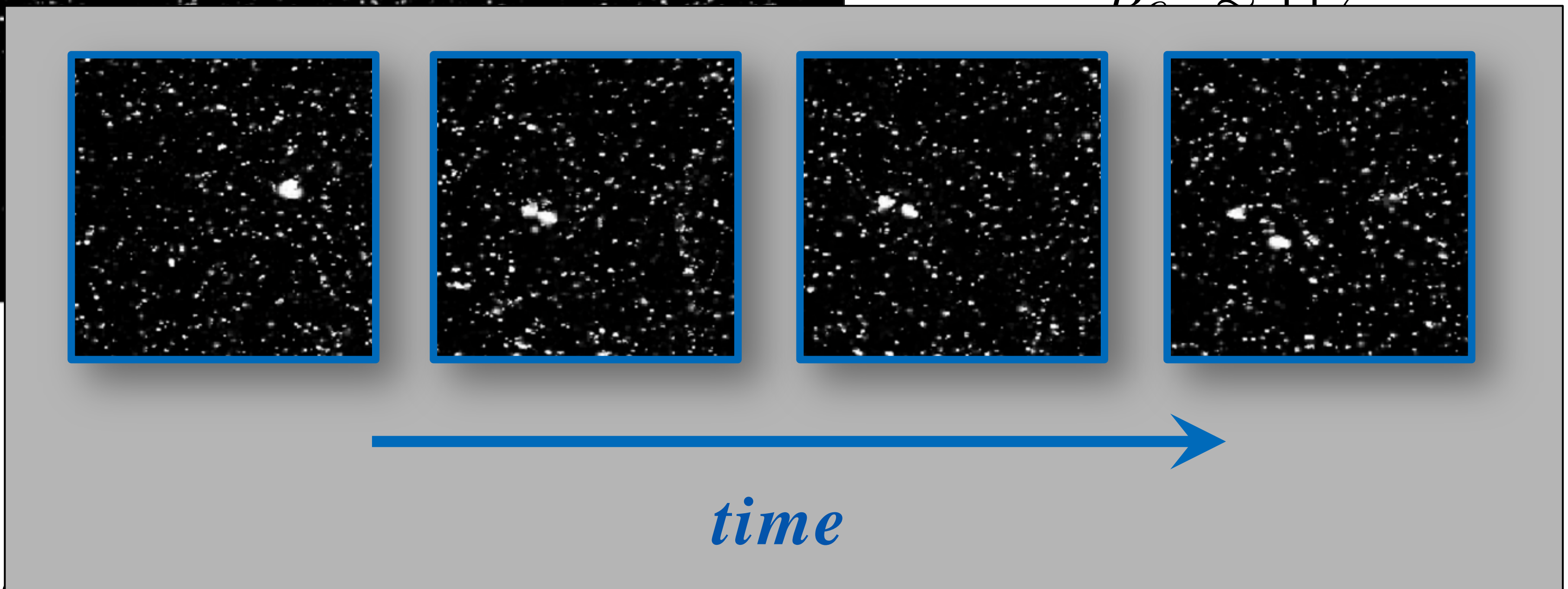

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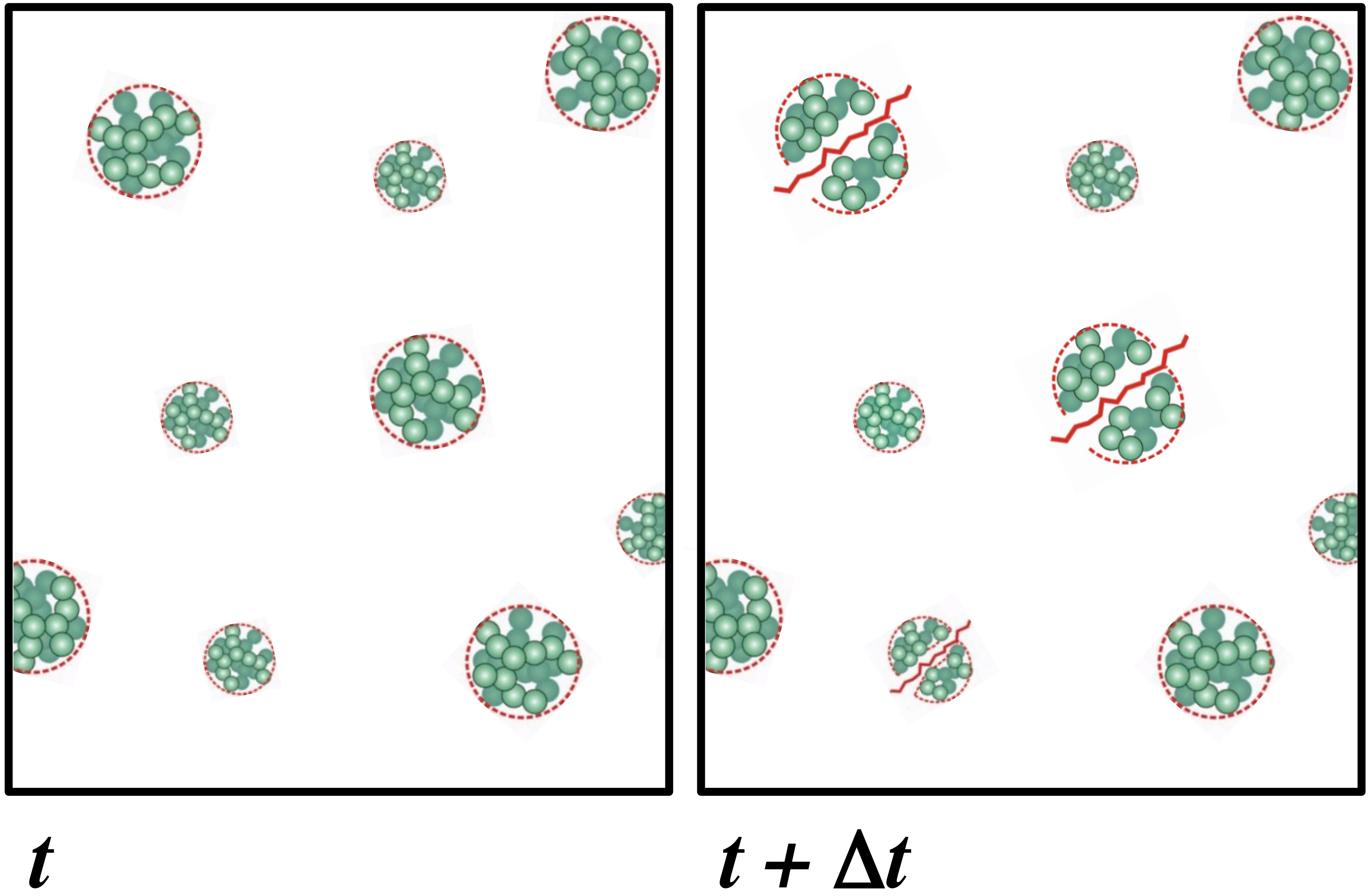
Aim and structure of this talk

Aim of this work:

Dynamics of breakup of small aggregates caused by turbulent fluid motions

$\sim$ *How many breakup events per unit time*



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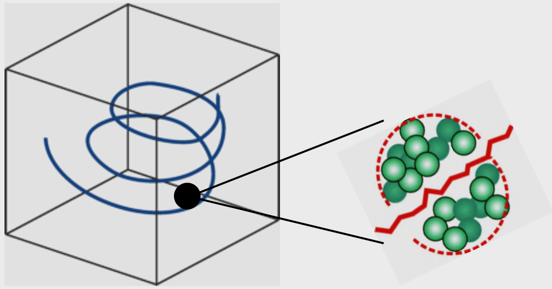
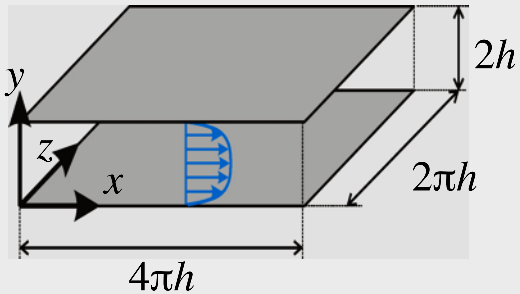
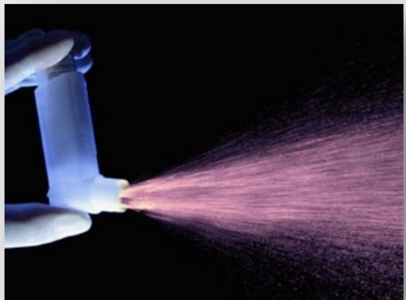


Colloidal aggregates in homogeneous isotropic turbulence



Colloidal aggregates in non-homogeneous flows



Aerosol aggregates in homogeneous isotropic turbulence

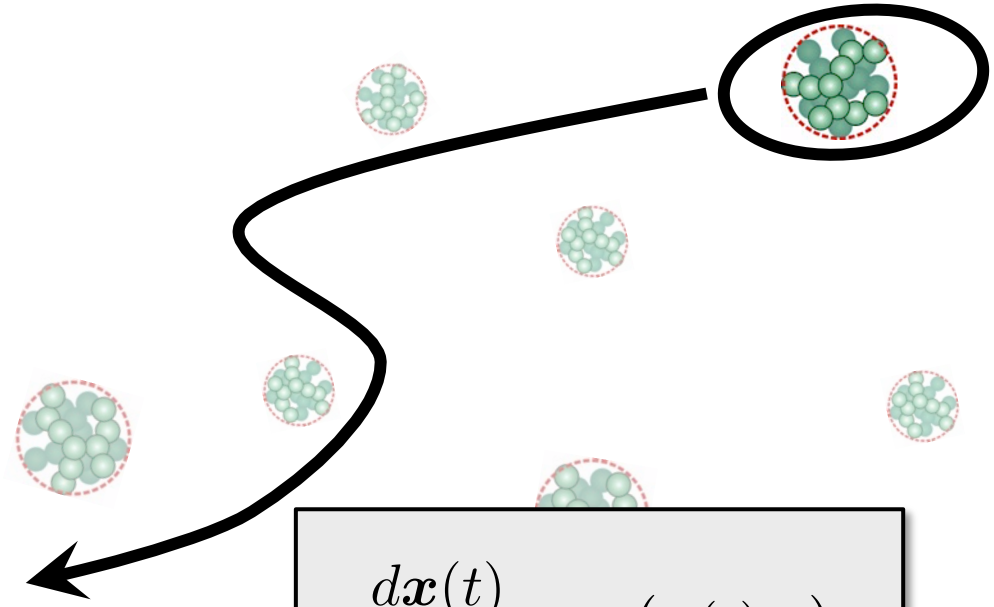
Numerical framework

- Stationary homogeneous isotropic turbulent flow, loaded with few aggregates

- Small colloidal aggregates
  - Aggregate size small with resect to η
  - Aggregate density close to fluid density

$R \ll \eta$

$\rho_a \sim \rho_f$



$$\frac{d\boldsymbol{x}(t)}{dt} = \boldsymbol{u}\big(\boldsymbol{x}(t), t\big)$$

Numerical framework

$$R \ll \eta$$

$$\rho_a \sim \rho_f$$

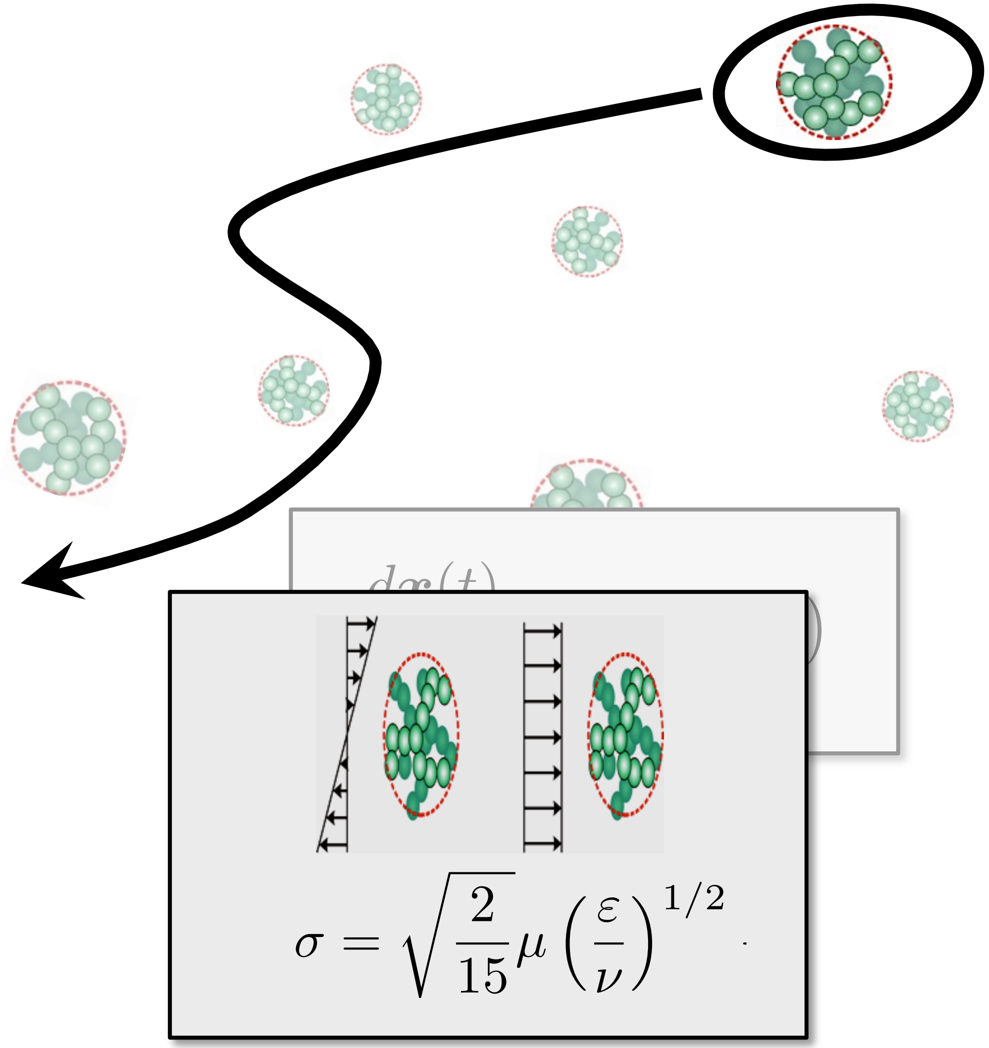
- Aggregates are broken due to due hydrodynamic stress acting on them

- *Brittle limit*: Aggregate break up when the hydrodynamic stress exceeds a critical value σ_{cr}

- σ_{cr} is a characteristic for a given type of aggregates

$$\sigma_{\rm cr} \sim R^{-1/q}$$

$$q \approx 0.35 - 0.55$$



Harshe *et al., Langmuir* (2011), Zaccone *et al.*, *PRE* (2009)

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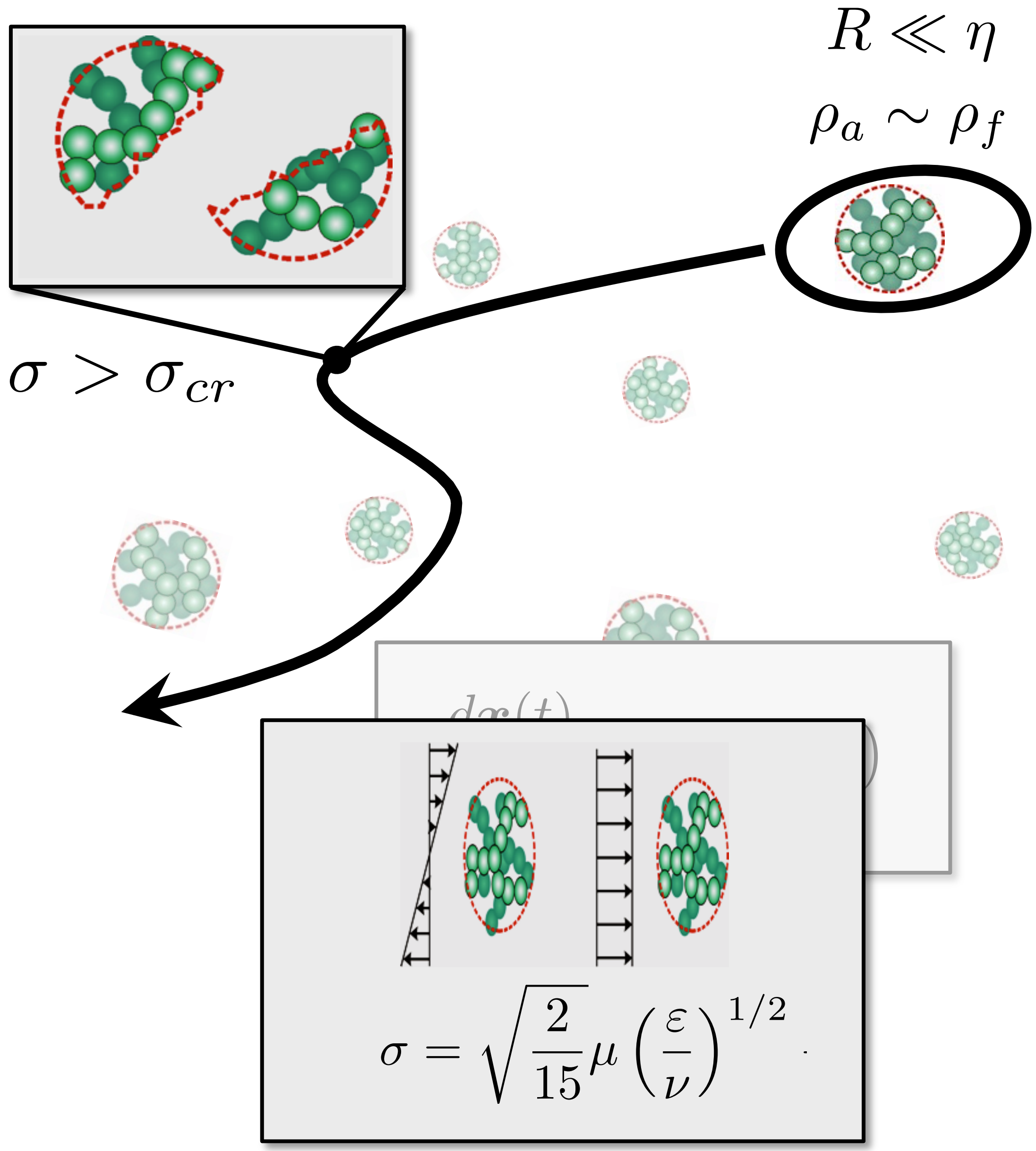
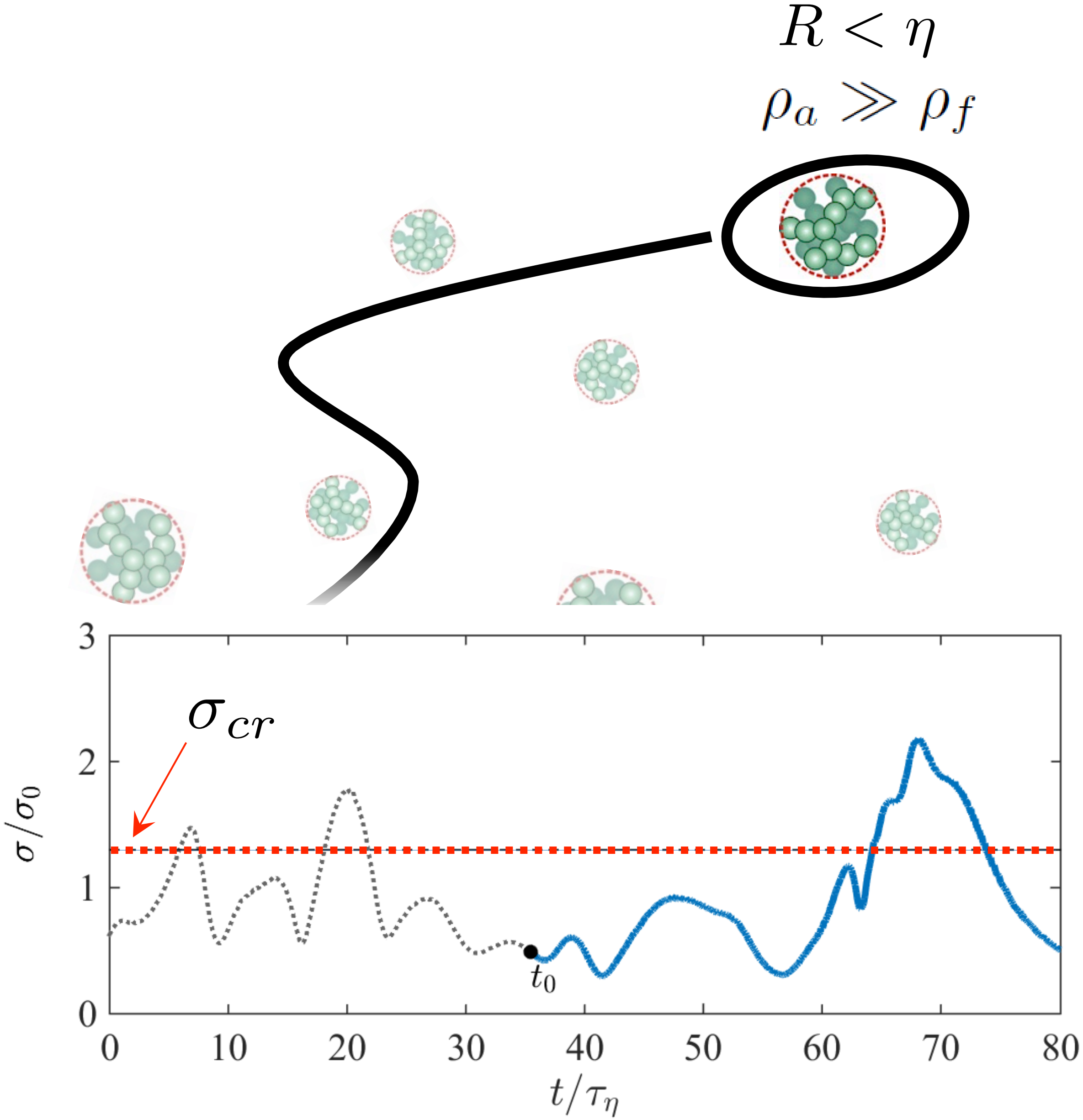


Harshe *et al.*, *Langmuir* (2011), Zaccone *et al.*, *PRE* (2009)

Numerical framework

- Upon release, we follow the aggregate until the first crossing of σ_{cr}



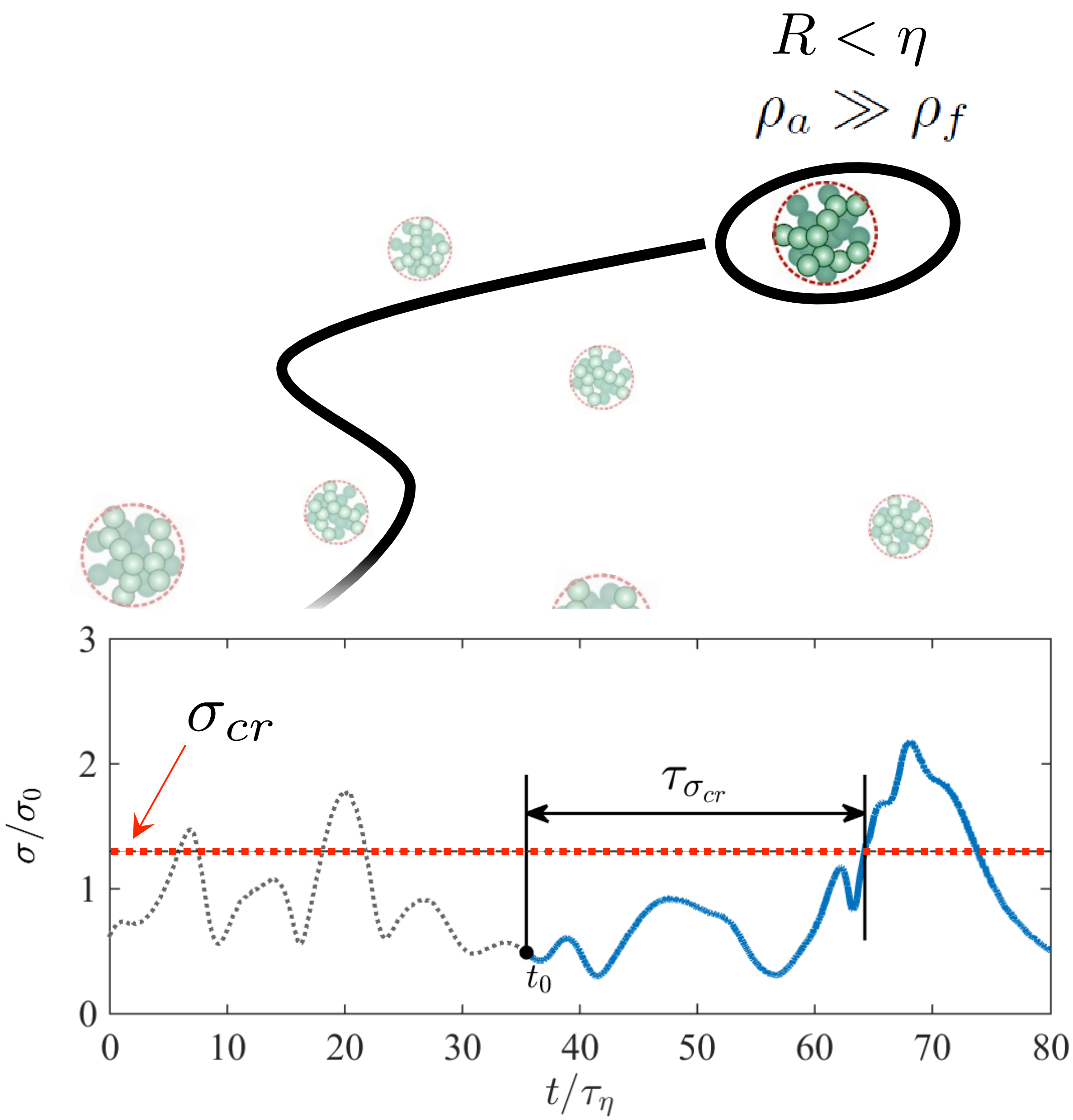
Babler, Biferale, Lanotte, *PRE* (2012)

Numerical framework

- Upon release, we follow the aggregate until the first crossing of σ_{cr}

- Breakup rate:

$$f_{\sigma_{\rm cr}} = \frac{1}{\langle \tau_{\sigma_{\rm cr}} \rangle}$$



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Numerical framework

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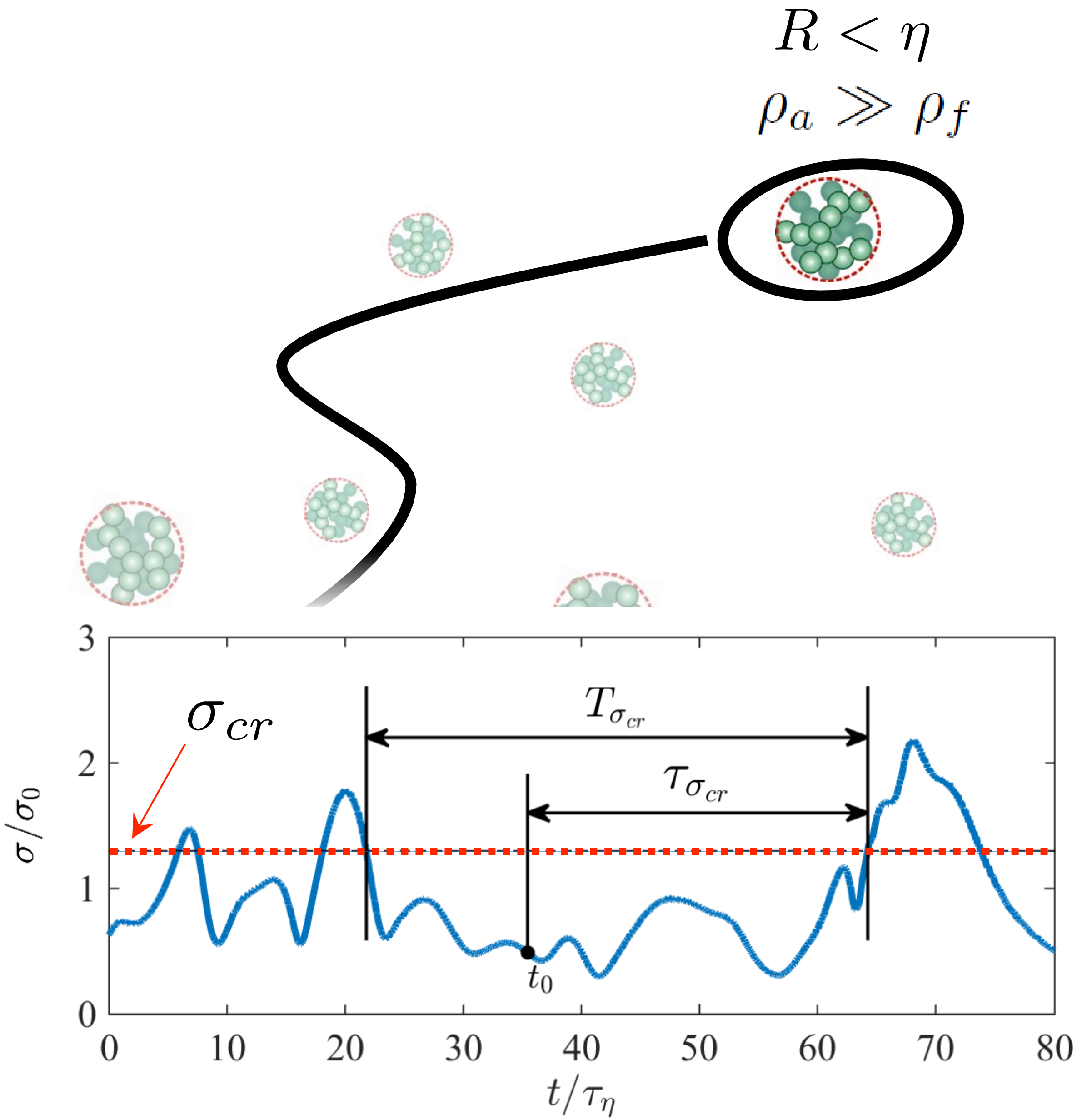
- Breakup rate:

$$f_{\sigma_{\rm cr}} = \frac{1}{\langle \tau_{\sigma_{\rm cr}} \rangle}$$

- Quasi-Eulerian proxy:

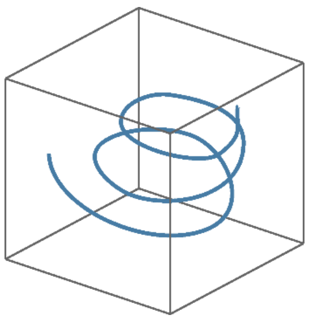
$$f^{(E)}_{\sigma_{\rm cr}} = \frac{1}{\langle T_{\sigma_{\rm cr}} \rangle} = \frac{\int_0^\infty d\dot\sigma\, \dot\sigma p_2(\sigma_{\rm cr}, \dot\sigma)}{\int_0^{\sigma_{\rm cr}} d\sigma\, p(\sigma)}$$



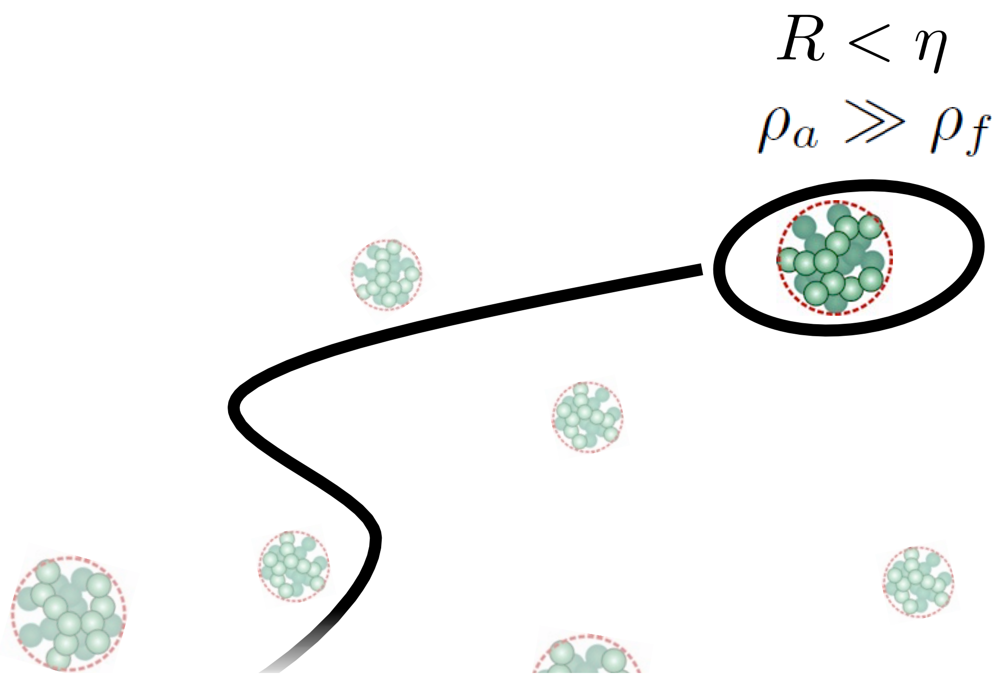
Babler, Biferale, Lanotte, *PRE* (2012)

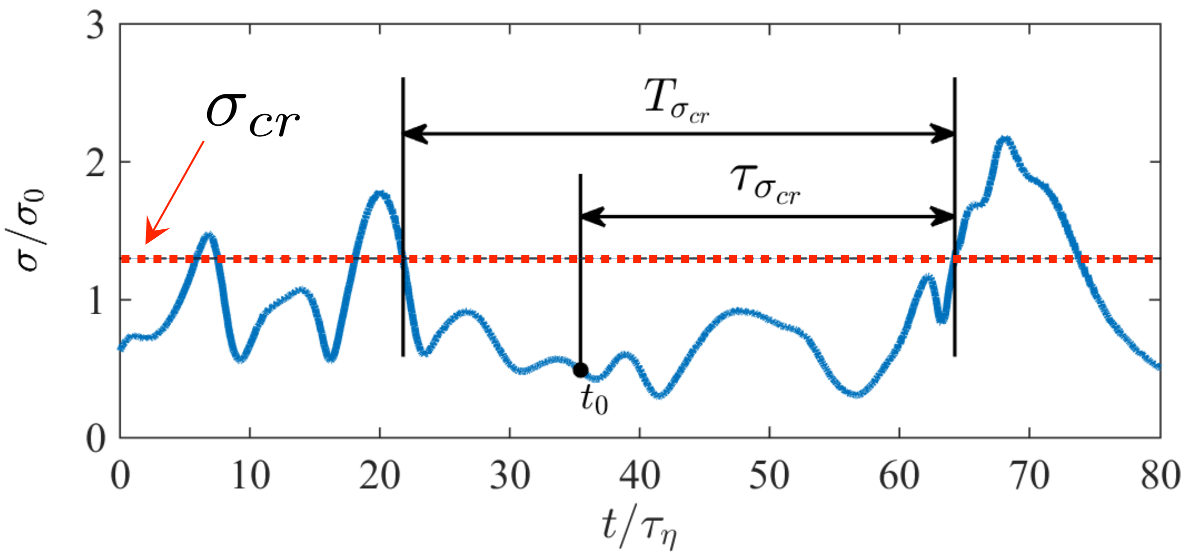
Numerical framework

- *Task*: Measure σ along turbulent trajectories and detect crossings of σ_{cr}
- Turbulent trajectories for HIT are available on http://turbase.cineca.it (as part of EuHIT program)



- Resolution 2048^3
- $Re_\lambda = 400$

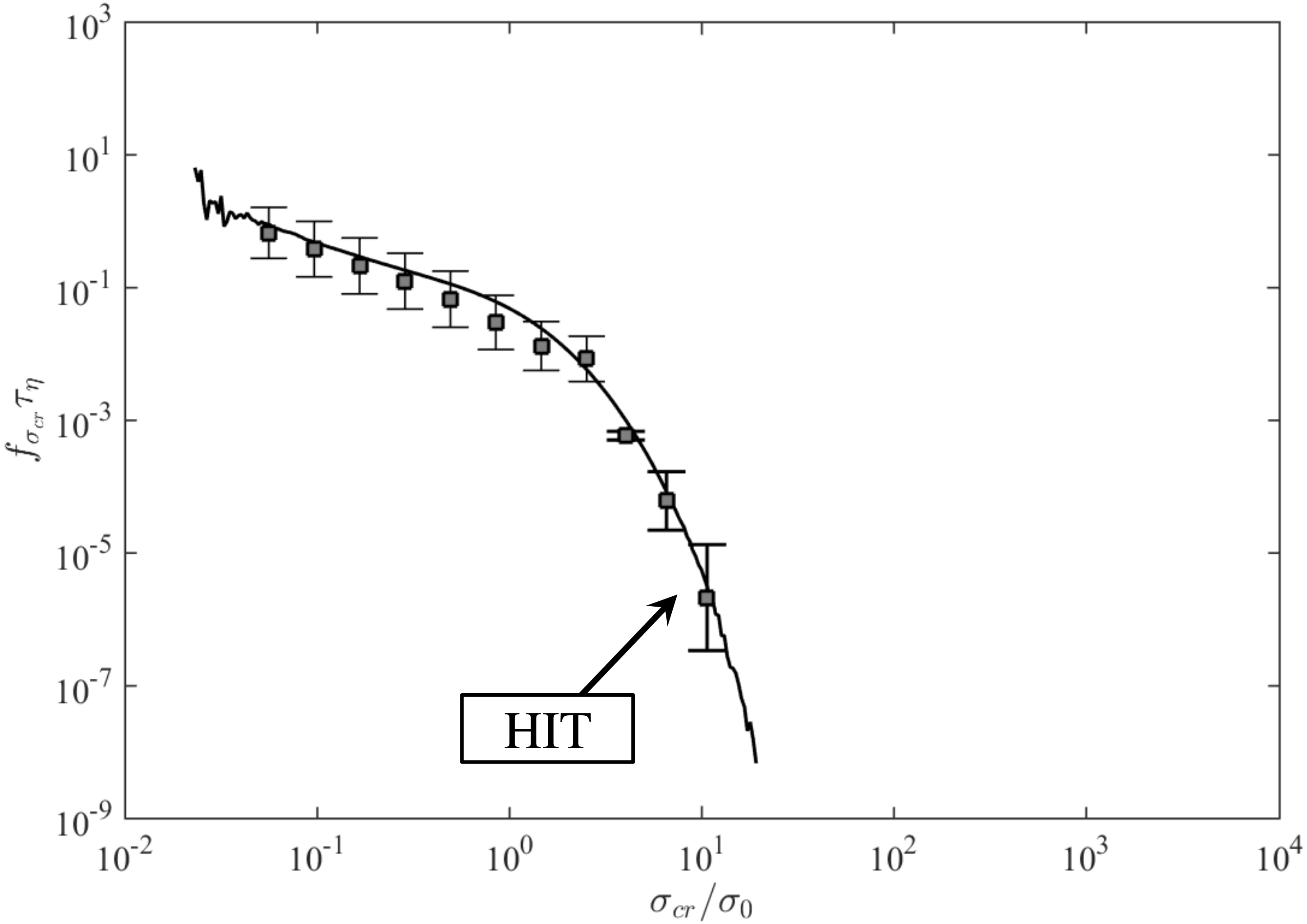




Babler, Biferale, Lanotte, *PRE* (2012)

Breakup rate I – Colloids/HIT

- Small colloidal aggregates ($R \ll \eta$, $\rho_a \sim \rho_f$)



Babler, Biferale, Lanotte, *PRE* (2012)

Breakup rate I – Colloids/HIT

- Small colloidal aggregates ($R \ll \eta$, $\rho_a \sim \rho_f$)

- Small thresholds

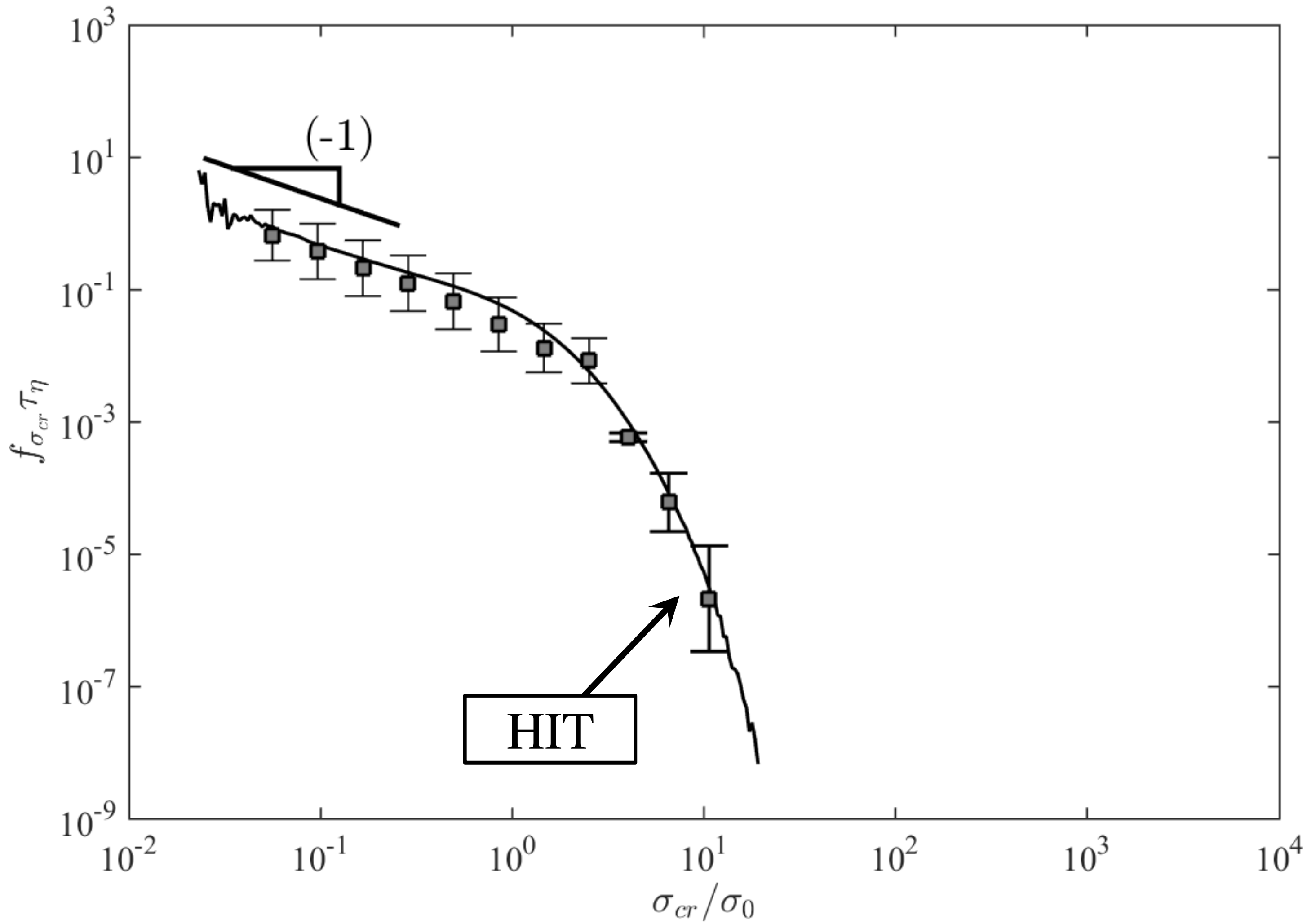
$$f^{(E)}_{\sigma_{\rm cr}} = \frac{\int_0^\infty d\dot\sigma\, \dot\sigma p_2(\sigma_{\rm cr}, \dot\sigma)}{\int_0^{\sigma_{\rm cr}} d\sigma\, p(\sigma)}$$

- Closure

$$p_2(\sigma, \dot\sigma) = p(\sigma)p(\dot\sigma)$$

$$p(\sigma) \sim \text{Gaussian}$$

$$\Rightarrow \quad f_{\sigma_{\rm cr}} \sim \sigma_{\rm cr}^{-1}$$



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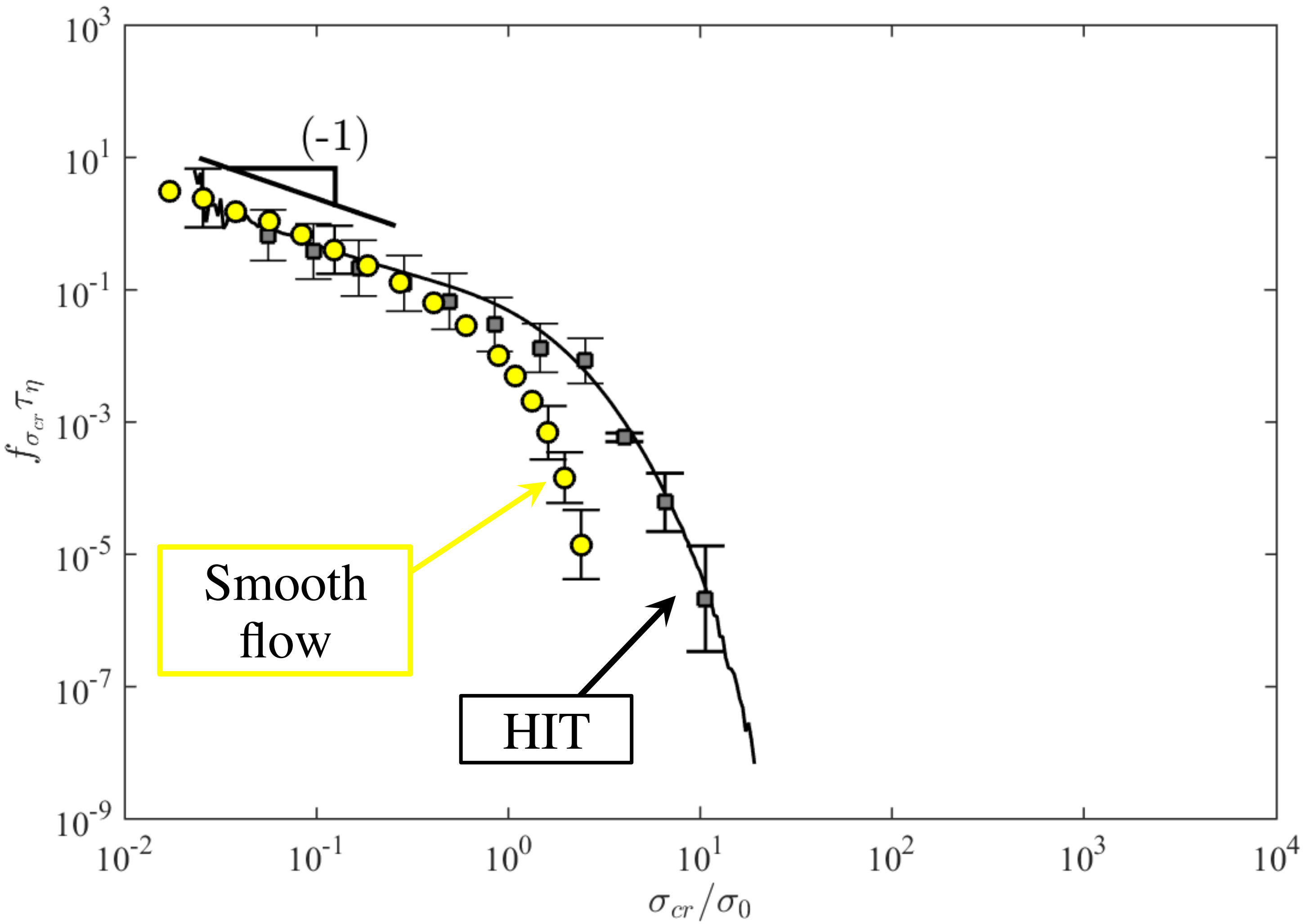
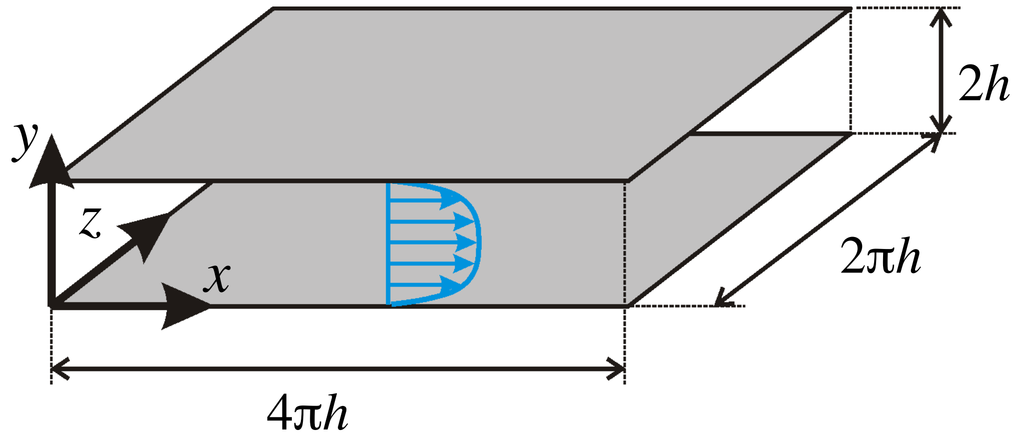


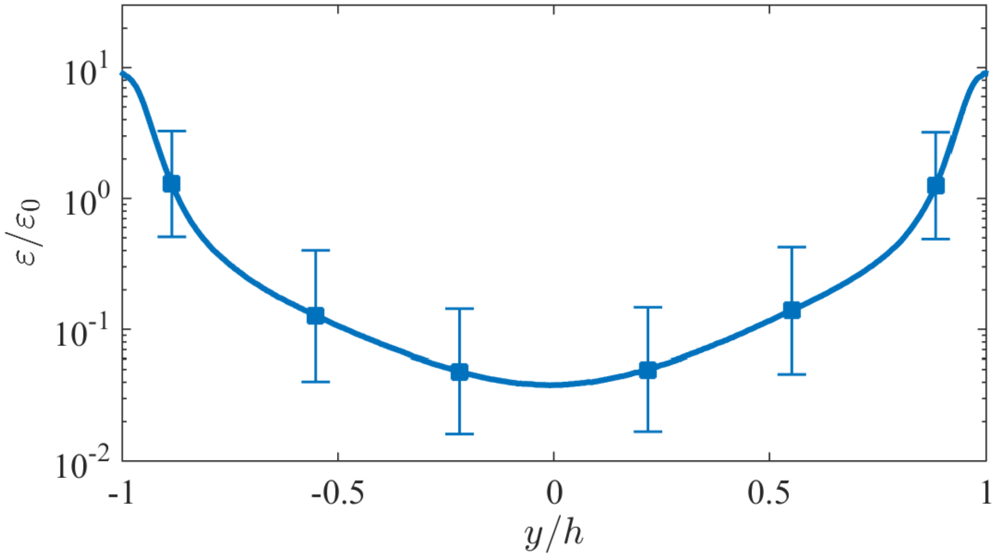
Babler, Biferale, Lanotte, *PRE* (2012), Babler *et al.*, *J. Fluid Mech.* (2015)

Colloidal aggregates in channel flow

- Stationary turbulent flow between two parallel plates
- Periodic in x and z,
  Resolution 128×128×129
- $Re_\tau = u_\tau h/\nu = 150$,
  $Re = 2Uh/\nu = 4200$

  u_τ = shear velocity,
  U = bulk velocity

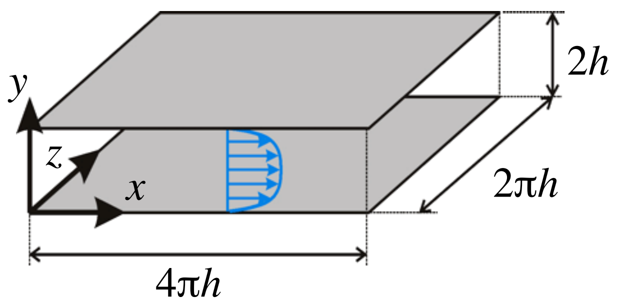


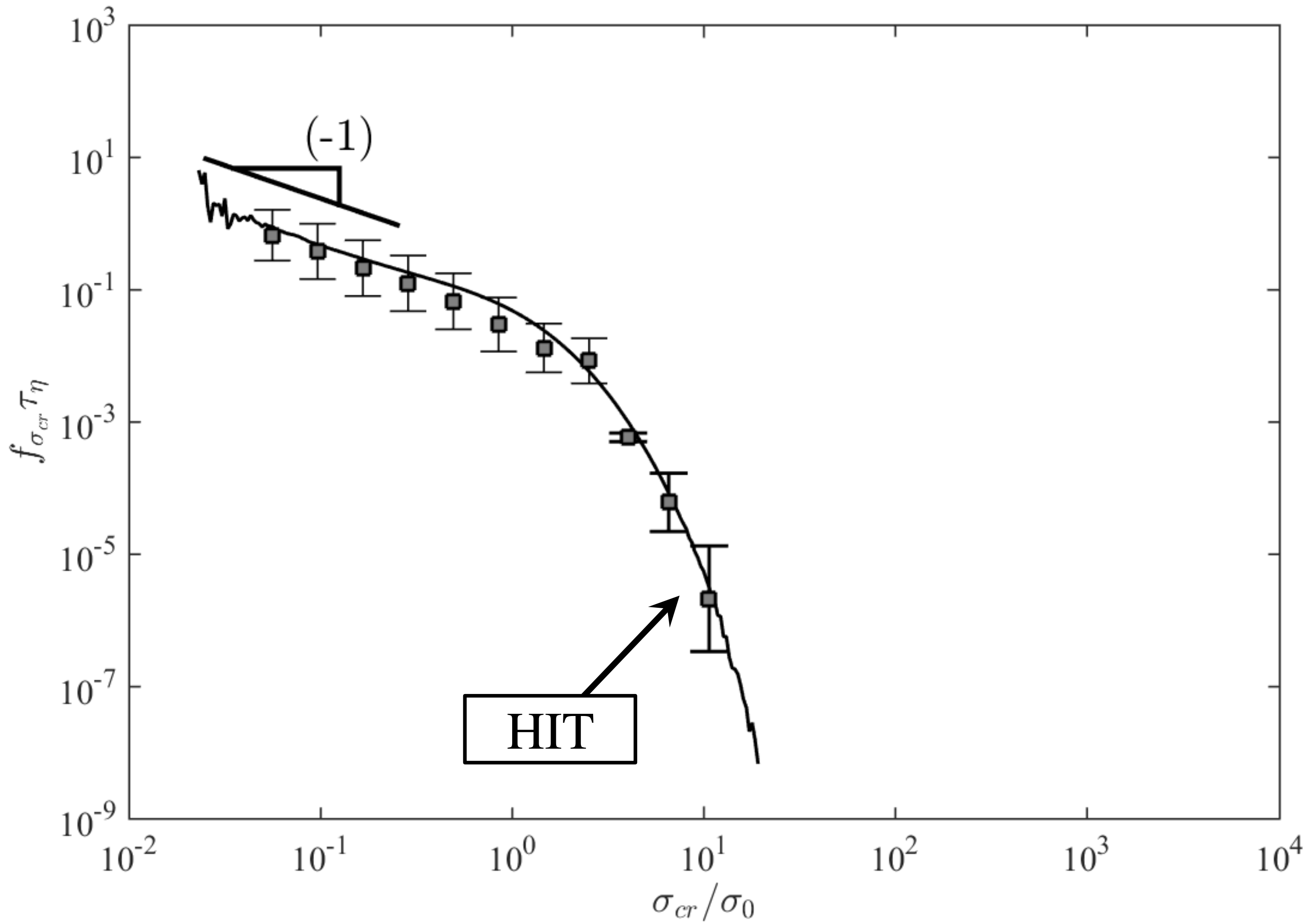


Marchioli and Soldati, *Intl. J. Muliphase Flow* (2009), Babler *et al.*, *J. Fluid Mech.* (2015)

Breakup rate II – Colloids/Channel

- Colloidal aggregates released in two locations:
  - Center-plane
  - Close to the wall





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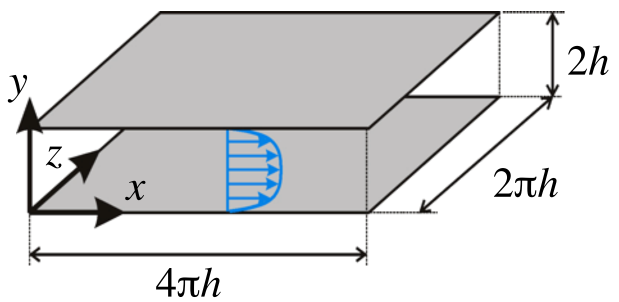

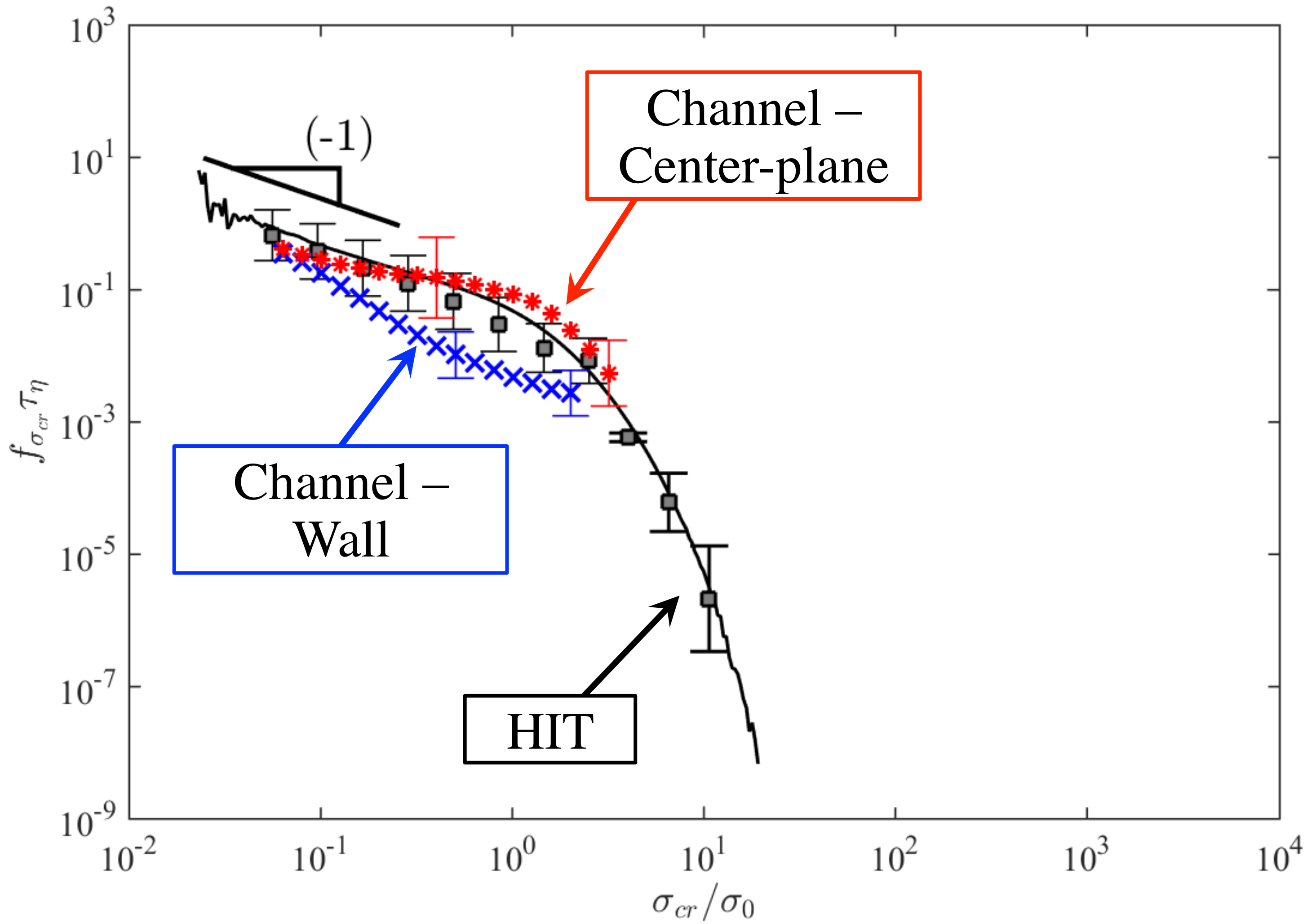

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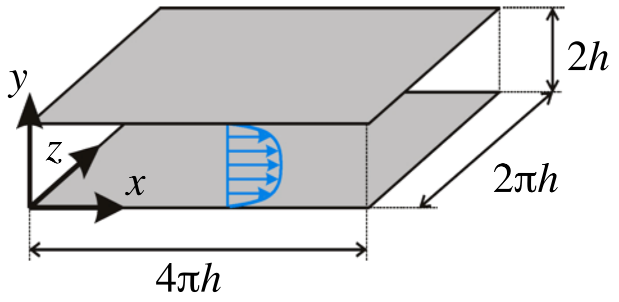
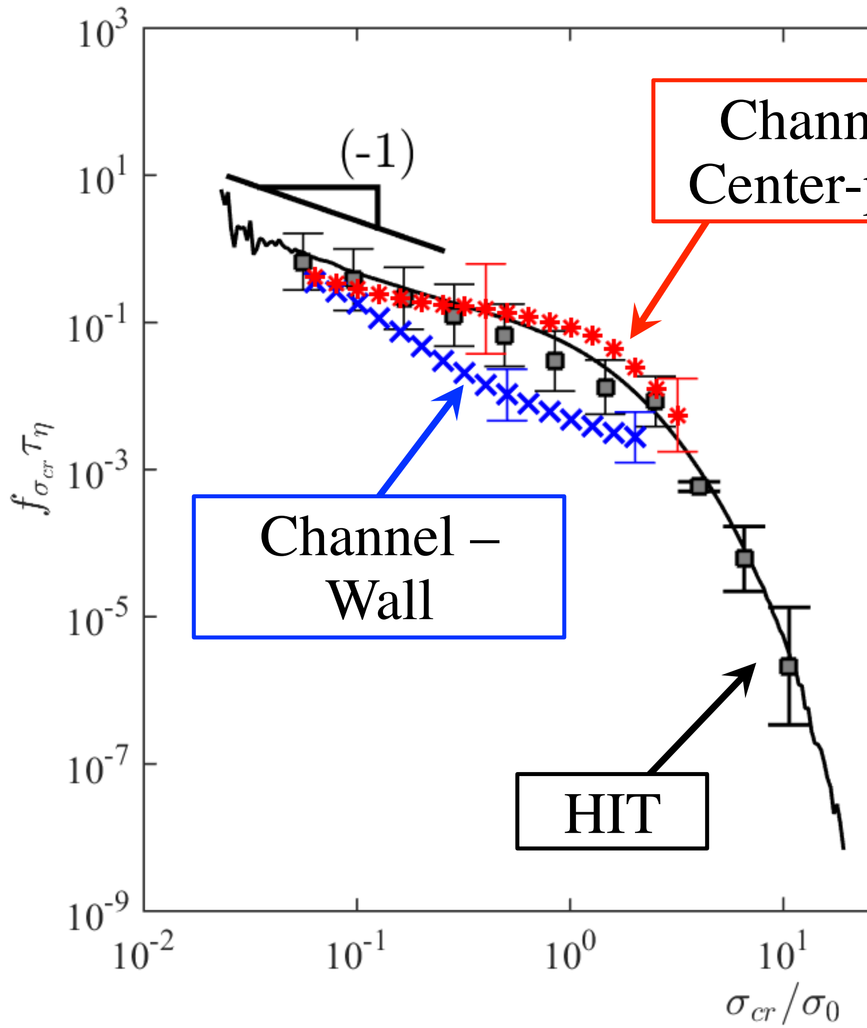
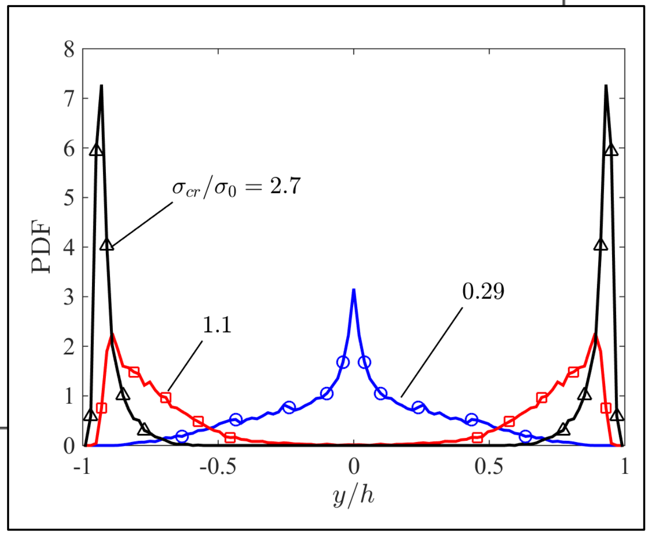


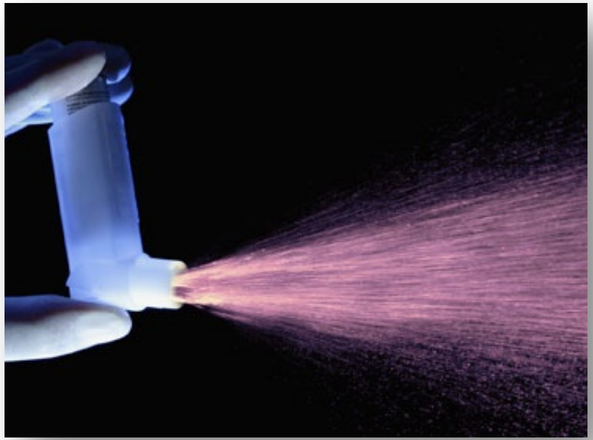




Location of breakup for release in the center-plane

Babler, *et al.*, *J. Fluid Mech.* (2015)

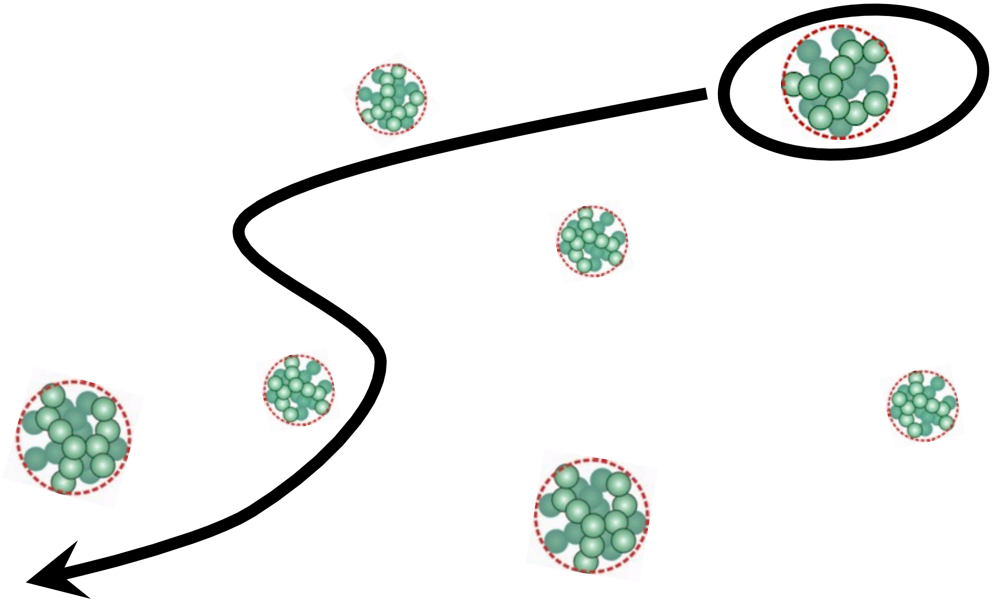
Aerosols in homogeneous turbulence



- Small & heavy aggregates:
  - Aggregate size small with resect to η
  - Aggregate density large with respect to fluid density

$$R < \eta$$

$$\rho_a \gg \rho_f$$



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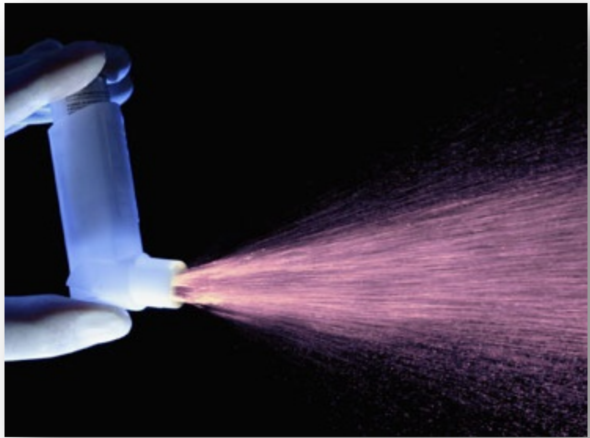

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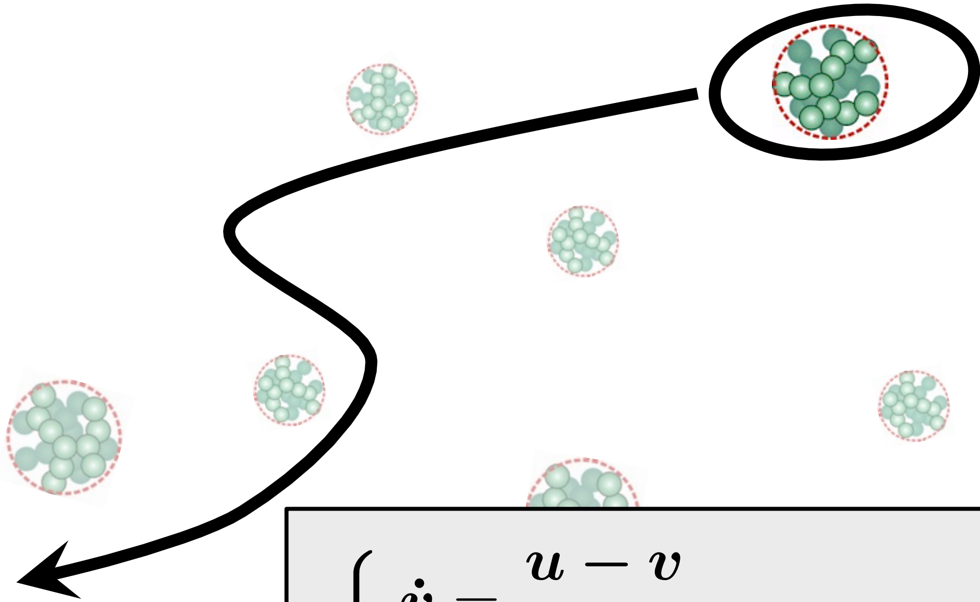


- Small & heavy aggregates:
  - Aggregate size small with resect to η
  - Aggregate density large with respect to fluid density

$$\begin{cases} \dot{\boldsymbol{v}} = \dfrac{\boldsymbol{u} - \boldsymbol{v}}{\tau_s} \\ \dot{\boldsymbol{x}} = \boldsymbol{v} \end{cases}$$

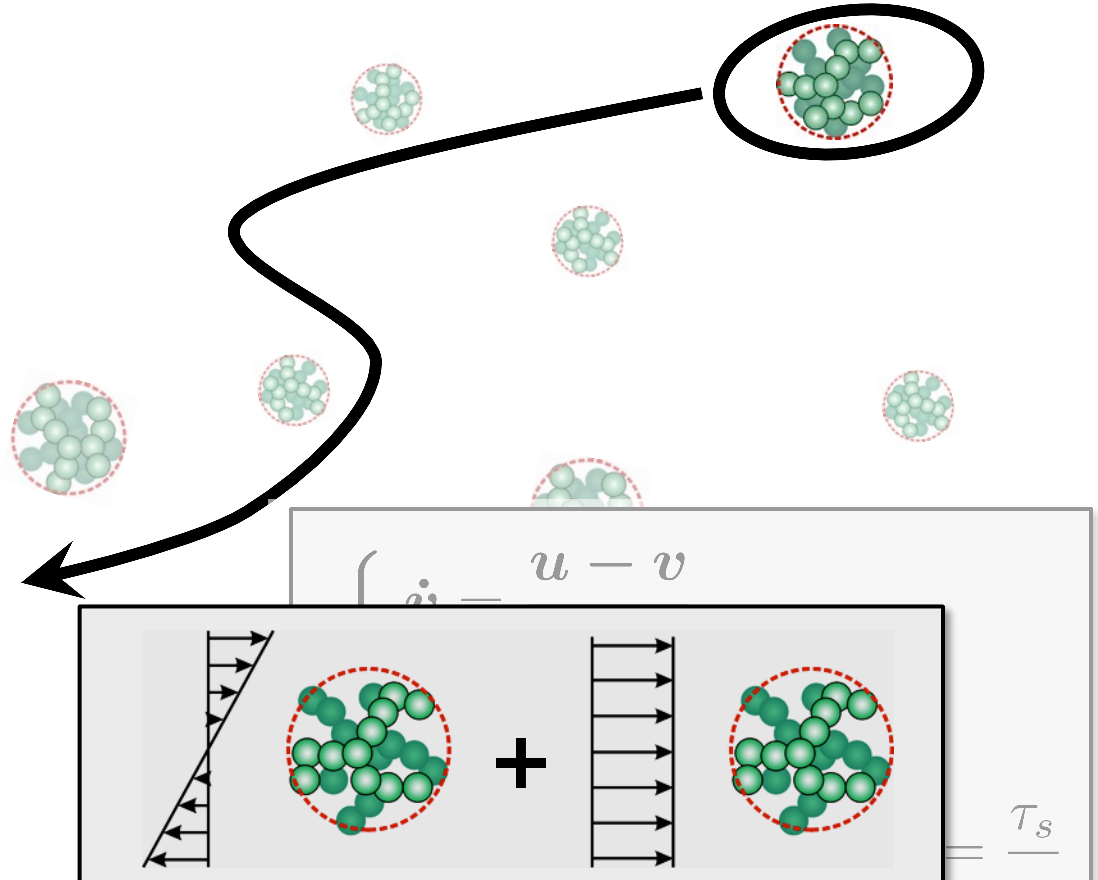
$$\tau_s = \frac{(2\rho_a + \rho_f)R^2}{9\rho_f \nu} \qquad St = \frac{\tau_s}{\tau_\eta}$$

Aerosols in homogeneous turbulence

$$R < \eta$$
$$\rho_a \gg \rho_f$$

- Hydrodynamic stress exerted on the aggregates is comprised of shear stress and drag stress

- *Brittle limit*: Aggregate break up when the hydrodynamic stress exceeds a critical value σ_{cr}



$$\sigma = \sqrt{\frac{2}{15}}\mu\left(\frac{\varepsilon}{\nu}\right)^{1/2} + \frac{3}{2}\mu\frac{|\boldsymbol{v}-\boldsymbol{u}|}{R}$$

K.A. Kusters (1991), Bagster and Tomi, *Chem. Eng. Sci.* (1974)

Aerosols in homogeneous turbulence

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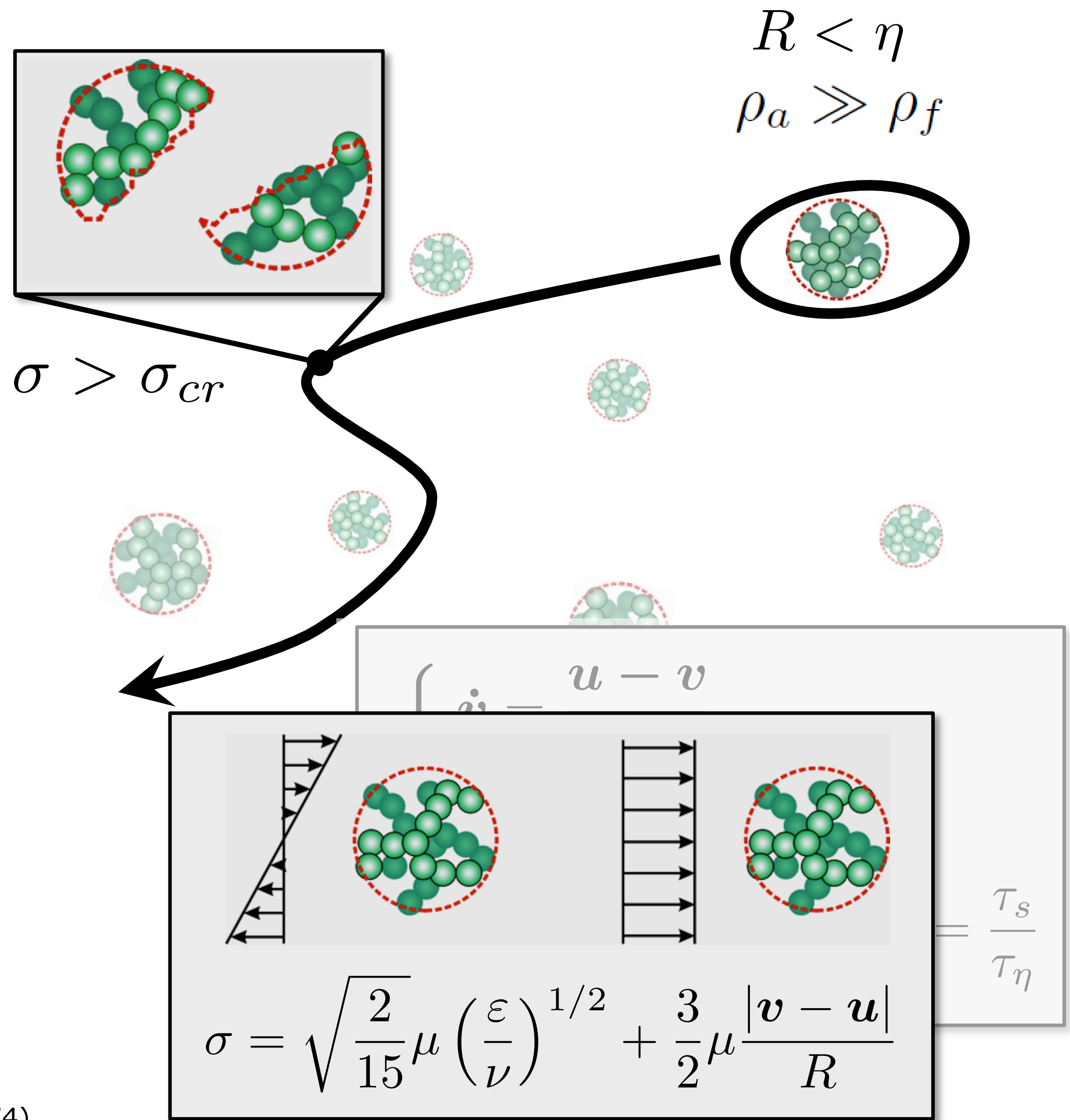
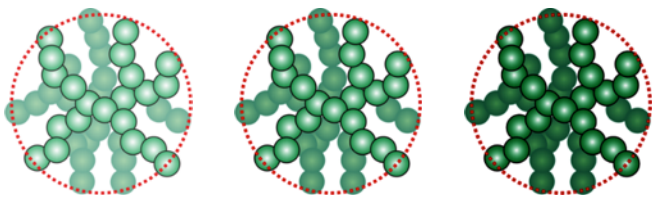
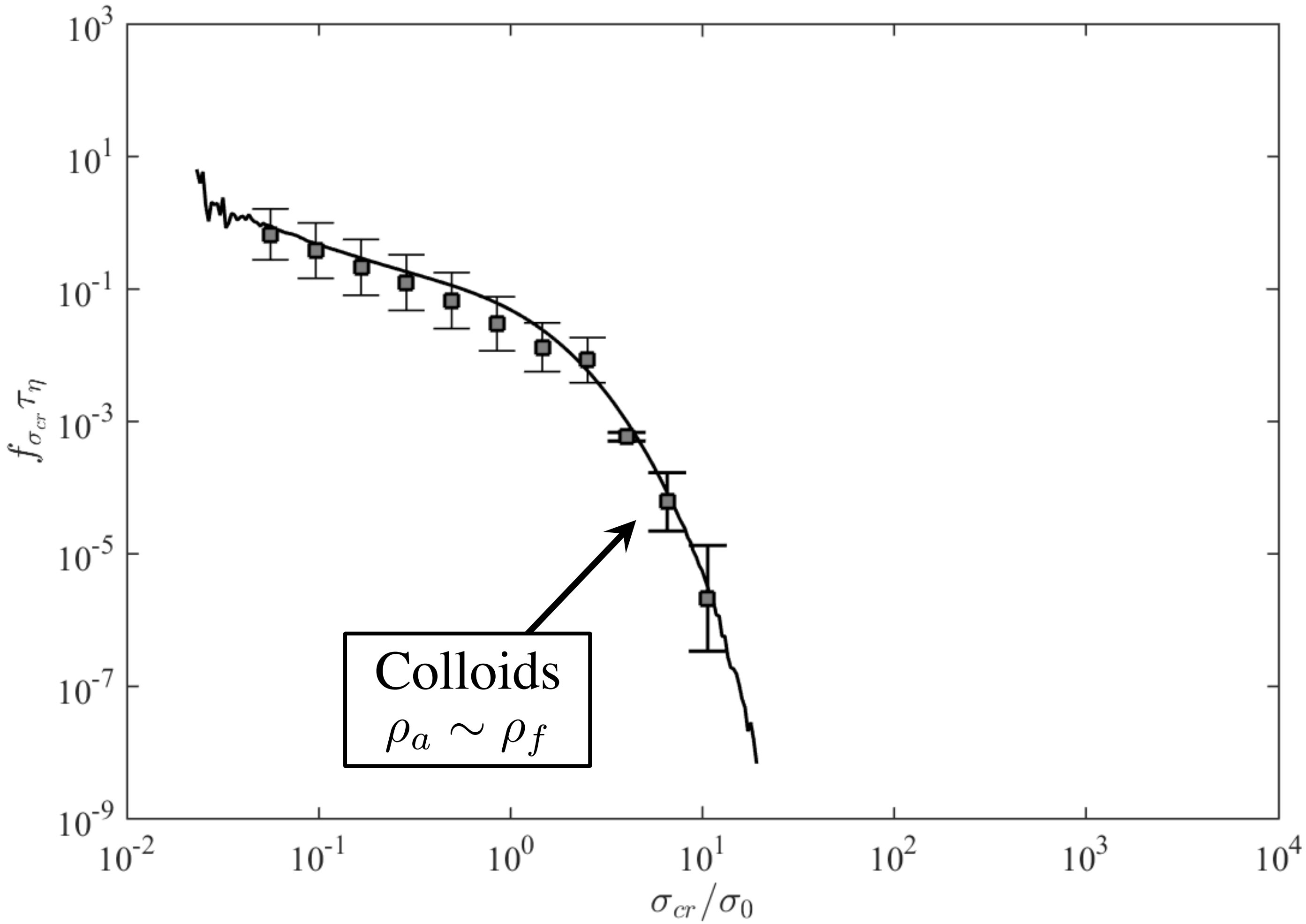


K.A. Kusters (1991), Bagster and Tomi, *Chem. Eng. Sci.* (1974)

Breakup rate III – Aerosols/HIT

- Aggregates of size $R/\eta = 0.1$ and varying density





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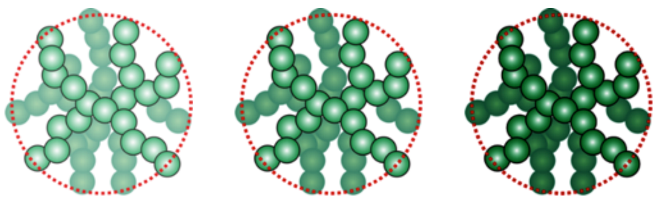

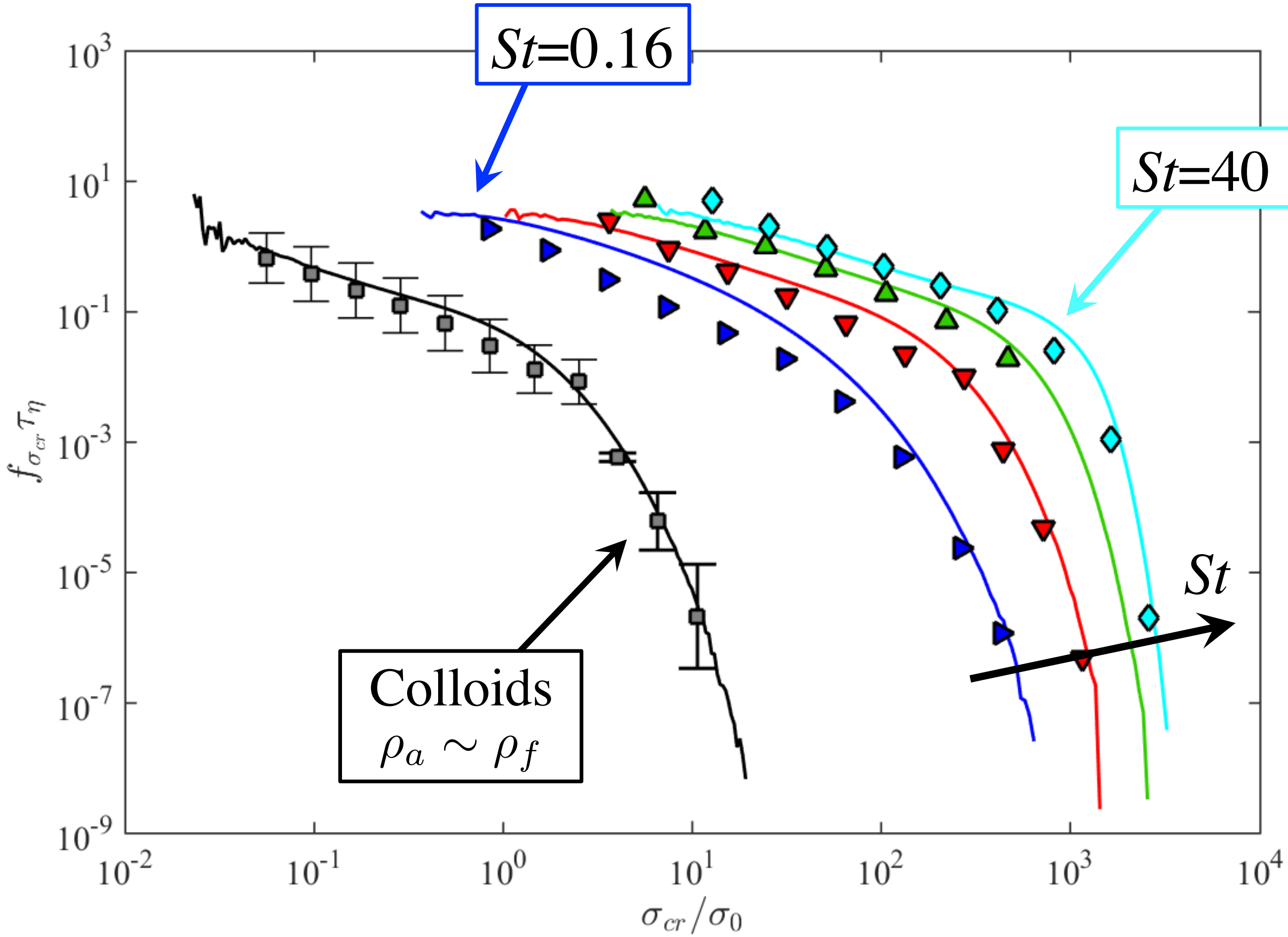

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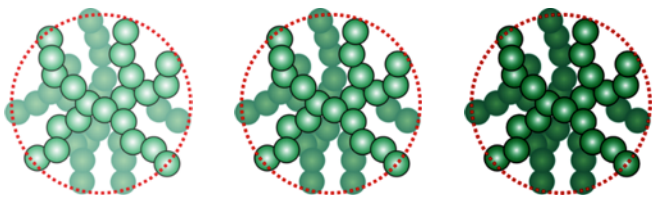

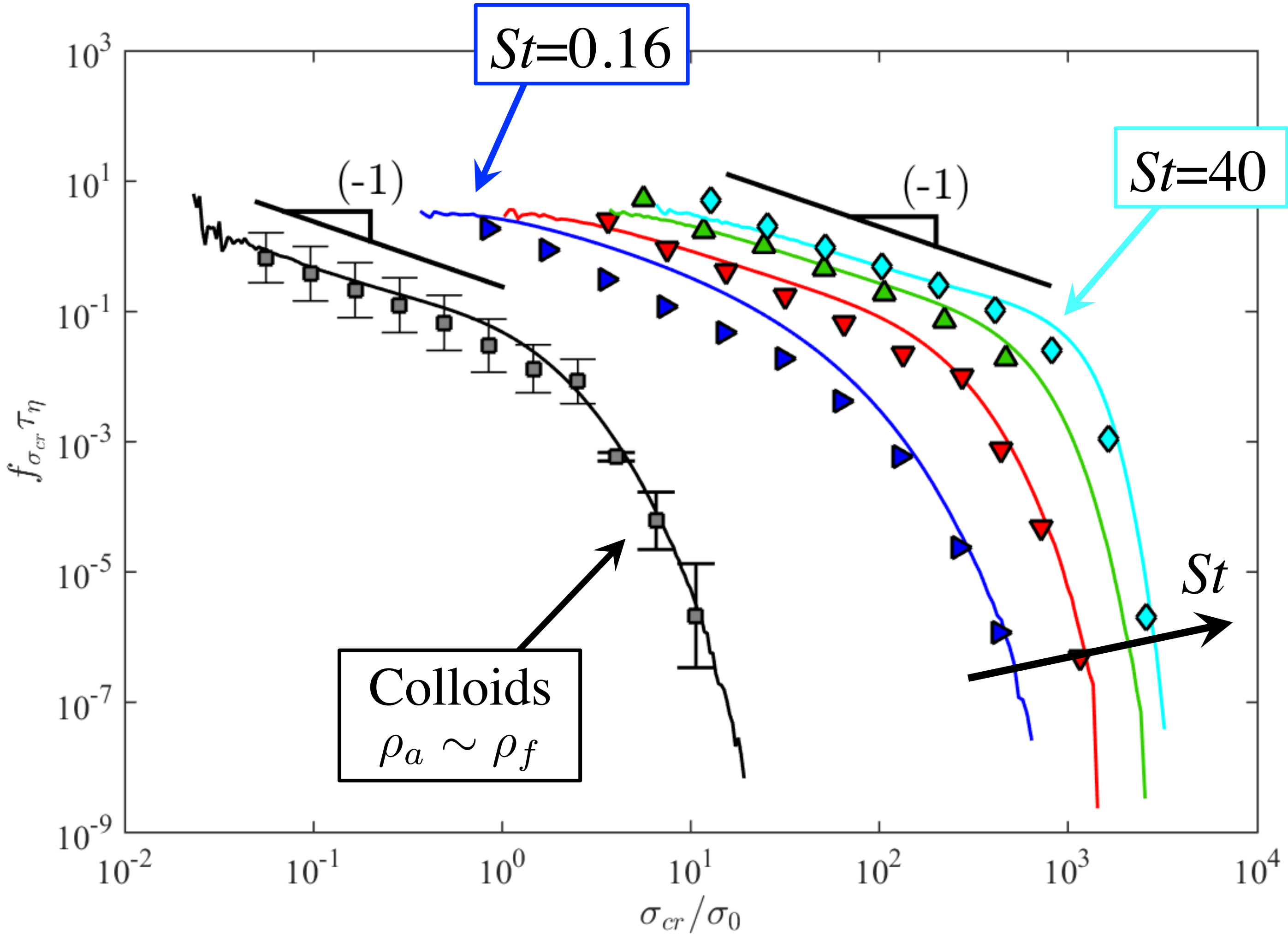

Conclusions

- We studied the breakup of colloidal and aerosol aggregates in different flow configurations. Breakup of an individual aggregate occurs instantaneously once the stress exceeds a critical threshold σ_{cr}. The latter depends on the aggregate properties such as size, structure, and nature of bonds. In this work σ_{cr} is used to characterize the aggregates.
- In all cases, the breakup rate as a function of σ_{cr} shows a power law-like behavior for small threshold values and a sharp cut-off for large threshold values. The former is caused by the calm parts of the flow while the latter is caused by rare intense fluctuations.
- In non-homogeneous flows we observe an intermediate regime in between small and large threshold values caused by transport of aggregates to the high shear zones close to the walls.
- Breakup of aerosol aggregates is influenced by drag stress. The drag stress increases with increasing the aggregate Stokes number.

Acknowledgements

- Swedish Research Council VR (M.U.B.)
- European Research Council ERC (L.B.)
- EU-COST Action MP1305 *Flowing Matter*